

Topological response theory of doped topological insulators

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We generalize the topological response theory of three-dimensional topological insulators (TI) to metallic systems – specifically, doped TI with finite bulk carrier density and a time-reversal symmetry breaking field near the surface. We show that there is an inhomogeneity-induced Berry phase contribution to the surface Hall conductivity that is completely determined by the occupied states and is independent of other details such as band dispersion and impurities. In the limit of zero bulk carrier density, this intrinsic surface Hall conductivity reduces to the half-integer quantized surface Hall conductivity of TI. Based on our theory we predict the behavior of the surface Hall conductivity for a doped topological insulator with a top gate, which can be directly compared with experiments.

Topological insulators (TI) are states of matter with a bulk energy gap and topologically protected gapless edge states. Their most striking properties are their topological responses, such as the quantized Hall conductance of integer quantum Hall (QH) states [1]. Recently, a wide class of time-reversal (TR) symmetry protected topological insulators has been discovered [2–5]. The three-dimensional ones are crystalline materials with a bulk energy gap and massless linearly dispersing Dirac-like surface states [6–8]. The topological responses of 3D TI can be observed when the surface states are gapped by magnetism [1] or superconductivity [10]. When the surface states are gapped by magnetism, the TI obtains a topological electromagnetic response described by the effective action $S_\theta = \frac{\theta}{2\pi} \frac{\alpha}{2\pi} \int d^3x dt \mathbf{E} \cdot \mathbf{B}$ with $\alpha = e^2/\hbar c$ the fine structure constant, and $\theta = \pi$ modulo 2π [1]. This is a topological magneto-electric effect and can be observed as a surface QH effect with a half integral quantized Hall conductivity $\sigma_{xy} = \frac{\theta}{2\pi} \frac{e^2}{h} = (n + \frac{1}{2}) \frac{e^2}{h}$, with n an integer. For non-interacting topological insulators θ can be calculated explicitly as the Chern-Simons invariant of the geometrical gauge field defined in momentum space [1, 11]. The topological response theory of 3D TI can be obtained by a dimensional reduction from the 4D generalization of the quantum Hall effect [12].

With the recent systematic understanding of topological insulators, a natural question is whether only insulators can be topological: are there topological phenomena in gapless systems such as a Fermi liquid? In this paper, we develop a theory to characterize the intrinsic response properties in a generic 3D Fermi liquid. Although in a metallic system the response properties such as Hall conductivity are not quantized, there can still be intrinsic “topological” contributions that are determined by the Berry phase gauge field in momentum space and are independent of non-topological details such as energy dispersion away from the Fermi surfaces and impurities.

An interesting example of a 3D Fermi liquid with non-trivial topological response is a doped TI—a system with the band structure of a TI but with a finite bulk car-

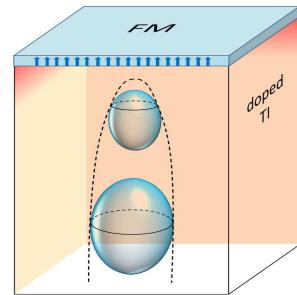


FIG. 1: Schematic picture of a doped TI with a ferromagnetic layer on the surface. The spheres indicate the Fermi surface size which is position dependent. Near the surface, the Fermi level lies in the gap.

rier density. Here, we study the surface Hall conductivity of a doped TI with TR breaking field applied at the surface, as illustrated in Fig. 1. (Some other behavior of doped TI inherited from the nearby TI has been studied recently [13, 14]). Unlike a TI, the surface Hall conductivity of a doped TI is not quantized, and is in general dependent on surface conditions. However, in the smooth boundary limit, where the changes of the Fermi level and the band structure near the boundary are smooth on the scale of the mean free path, we show that the surface Hall conductivity is determined by a topological invariant—the Chern-Simons invariant of the geometrical gauge field integrated over the two-dimensional Fermi surface and the real space direction perpendicular to the boundary. We obtain our result by generalizing the dimensional reduction approach in Ref. [1] to metallic systems. Our result can be understood as a higher dimensional, inhomogeneity-induced generalization of the intrinsic anomalous Hall effect [15–18] and its interpretation as a topological property of Fermi liquids [19]. Our results for doped TI are relevant to the current experiments on TI materials since all the known 3D TI materials, such as $\text{Bi}_{1-x}\text{Sb}_x$ alloy [20, 21], Bi_2Se_3 and Bi_2Te_3 [22–24], have finite residual carrier density, which has become a major experimental challenge for the observation of topological effects in TI. We also nu-

merically studied the surface Hall conductivity of doped Bi_2Se_3 with a simple surface T-breaking field using the four band effective model [22, 25]; our results can be verified by zero-field transverse conductance measurements of Bi_2Se_3 with a magnetic layer deposited on the surface and voltage applied at a top gate.

Consider a Hamiltonian $H_{3D}[A_\mu, \theta(\mathbf{r})]$ for a 3+1D non-interacting fermion system that is coupled to the electromagnetic gauge field A and that depends on a spatially varying parameter $\theta(\mathbf{r})$. For example, in a doped TI with a boundary, $\theta(\mathbf{r})$ may describe both the spatial variation of the Fermi energy and the change of band structure across the boundary. Without losing generality, we can define $\theta = 0$ and π to describe the vacuum and the bulk of the doped TI, respectively. To study the surface of a doped TI, we take $\theta(\mathbf{r}) = \theta(z)$ to depend on one direction of space, with $\theta(z \rightarrow -\infty) = \pi$ deep in the bulk, while $\theta(0) = 0$ at the surface. When θ varies smoothly, at each point in space the system without external magnetic field is locally described by a Bloch Hamiltonian $H = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger h[\mathbf{k}, \theta(z)] c_{\mathbf{k}}$, where $\mathbf{k} = (k_x, k_y, k_z)$. For N bands, $c_{\mathbf{k}}$ is a N -dimensional vector and $h[\mathbf{k}, \theta(z)]$ is a $N \times N$ Hermitian matrix. In the physical system θ is defined in the region $[0, \pi]$. It is convenient to extend the definition of $h[\mathbf{k}, \theta]$ to $\theta \in [0, 2\pi]$ by setting $h[\mathbf{k}, \theta] = T^\dagger h[-\mathbf{k}, 2\pi - \theta] T$ for $\pi \leq \theta \leq 2\pi$. Here T is the time-reversal operator, and $h[\mathbf{k}, \theta]$ is continuous in θ since it is TR invariant at $\theta = 0, \pi$.

Now we study the electromagnetic response of the system, which is determined by the effective action

$$e^{iS_{\text{eff}}[A_\mu, \theta]} = \int \mathcal{D}\bar{c} \mathcal{D}c e^{i \int dt [\sum_i \bar{c}_i i \partial_t c_i - H_{3D}[A, \theta]]}. \quad (1)$$

The DC Hall conductivity is determined by the quadratic term in the action:

$$S_{\text{eff}}^{\text{Hall}}[A_\mu, \theta] = \frac{1}{2} \int d^3x dt \epsilon^{\mu\nu\sigma\tau} \sigma_\mu[\theta] A_\nu \partial_\sigma A_\tau. \quad (2)$$

with the Greek letters $\mu, \nu, \dots = 0, 1, 2, 3$ labeling the time and space coordinates. The spatial components σ_i , $i = 1, 2, 3$ of the four vector σ_μ are the Hall conductivity in yz , zx and xy plane, respectively; that is, $\sigma_i = \epsilon^{ijk} \sigma_{jk}$, with σ_{jk} the conductivity tensor. In general, $\sigma_i = \sigma_i[\theta(\mathbf{r})]$ is a functional of the inhomogeneous $\theta(\mathbf{r})$. For a smooth function $\theta(\mathbf{r})$, one can expand $\theta(\mathbf{r}) = \theta_0 + \mathbf{r} \cdot \nabla \theta(\mathbf{r})|_{\mathbf{r}=0}$ with $\theta_0 = \theta(\mathbf{r} = 0)$. In this expansion σ_i can be expanded to [31]

$$\sigma_i[\theta(\mathbf{r})] \simeq C_{1i}(\theta_0) + \frac{1}{2\pi} G_3(\theta_0) \partial_i \theta. \quad (3)$$

The coefficients in the two terms are given by two-point and three-point correlation functions, respectively. Using the time-ordered Green's function $G(\mathbf{k}, \omega) =$

$[\omega - e^{-i\delta} h(\mathbf{k})]^{-1}$, the coefficients can be expressed as:

$$C_{1i}(\theta_0) = \frac{1}{8} \int \frac{d^3 k d\omega}{(2\pi)^3} \epsilon^{ijkl} \text{Tr} [G \partial_j G^{-1} G \partial_k G^{-1} G \partial_l G^{-1}] \quad (4)$$

$$G_3(\theta_0) = -\frac{i\pi^2}{3} \epsilon^{ijkl} \int \frac{d^3 k d\omega}{(2\pi)^5} \text{Tr} [G \partial_i G^{-1} G \partial_j G^{-1} \cdot G \partial_k G^{-1} G \partial_l G^{-1} G \partial_\theta G^{-1}]. \quad (5)$$

with $\partial_j = \partial/\partial k_j$ and k_j is the frequency and momentum vector with $k_0 = \omega$ the frequency and $(k_1, k_2, k_3) = \mathbf{k}$ the momentum.

Before evaluating the correlation functions, let us discuss the criteria for the validity of the above effective theory approach. In the case of a band insulator with a gap E_g , there is a length scale $\xi = \hbar v/E_g$ where v is a typical velocity scale contained in the coupling between conduction and valence bands. The approach above is valid as long as the characteristic scale of variations of θ is much longer than ξ , i.e., $|\nabla \theta| \ll 1/\xi$. For a perfect metal, the gap vanishes and the Green's function in (4) and (5) is singular. With impurities, the Green's function obtains a finite self-energy $1/\tau$, which corresponds to a length scale $l = v_F \tau$, which is the mean-free path. The mean-free path plays the role of ξ in the insulator case, and the expansion above applies to the system with $|\nabla \theta| \ll 1/l$. Physically, the expansion applies because the conductivity at position \mathbf{r} will be insensitive to small changes in θ that occur at \mathbf{r}' when $|\mathbf{r}' - \mathbf{r}| \gg l$. In other words, the intrinsic contribution to the Hall conductivity calculated above applies in the “dirty limit” where the Hamiltonian is smoothly varying on the scale of the mean-free path, although the value of the intrinsic Hall conductivity is independent of the impurity strength in this limit. In general, the anomalous Hall conductivity of a metal also receives extrinsic contributions arising from impurity scattering, which are termed the side-jump and skew-scattering contributions [18]. Here we focus on the intrinsic contributions, which depend only on the nature of the Bloch states and their associated Berry phases. In the case of ferromagnetic metals, the intrinsic contribution can dominate the full anomalous Hall conductivity in certain intermediate regimes of disorder [18]; thus we expect that the intrinsic contribution that we calculate here for the surface of a doped TI may also be the dominant contribution in certain regimes of disorder.

Under the condition discussed above, the gradient expansion can be done locally around each point in space, leading to a local Hall conductivity. For simplicity, we consider $\theta(\mathbf{r}) = \theta(z)$ only varying along the z direction. The Hall conductivity in the xy plane is given by $\sigma_z(z) = C_1^z[\theta(z)] + \frac{G_3}{2\pi}[\theta(z)] \partial_z \theta(z)$. As shown in Fig. 1, we consider a single interface at $z = 0$ between the vacuum at $z > 0$ and a doped topological insulator at $z < 0$. One can always take $\theta = -\pi$ for the bulk doped TI and $\theta = 0$ for the vacuum, both of which are TR

invariant. In such a situation, the total current in the xy -plane will be given by $j_{2D}^\mu = \int dz j^\mu$, from which we may obtain the two-dimensional Hall conductivity $\sigma_z^{2D} = \int dz \sigma_z(z) = \sigma_z^{2D;(1)} + \sigma_z^{2D;(2)}$. The first term $\sigma_z^{2D;(1)} = \int dz C_{1z}[\theta_0(z)] = \frac{1}{4\pi^2} \sum_\alpha \int d^3k dz \mathcal{F}_{xy}^\alpha(z) n_\alpha(\mathbf{k}, z)$ is the intrinsic anomalous Hall conductivity of a homogeneous system[15, 16], where α labels the occupied bands $|\alpha\mathbf{k}\rangle$, and n_α and \mathcal{F}_{xy}^α are the occupation number and Berry curvature of band α . More explicitly $\mathcal{F}_{xy}^\alpha = \partial_x A_y^\alpha - \partial_y A_x^\alpha$ with $A_i^\alpha = -i \langle \alpha\mathbf{k} | \partial_{k_i} | \alpha\mathbf{k} \rangle$. Modulo a quantized contribution $n/2\pi$ with integer n , $\sigma_z^{2D;(1)}$ is determined by the Berry phase gauge field at the Fermi surface[19]. The second term $\sigma_z^{2D;(2)} = \frac{1}{2\pi} \int dz G_3[\theta_0(z)] \partial_z \theta = \frac{1}{2\pi} \int_{-\pi}^0 G_3(\theta) d\theta$ is the new contribution induced by spatial inhomogeneity. With TR symmetry only broken at the interface, one can extend the definition of θ to $[0, 2\pi]$ as mentioned above. By TR symmetry it can be proved that $G_3(\theta) = G_3(-\theta)$, so that $\int_0^\pi d\theta G_3(\theta) = \frac{1}{2} \int_0^{2\pi} d\theta G_3(\theta)$.

Therefore, as long as the start and end points are described by time-reversal invariant Hamiltonians, we find that the integrated current response receives a contribution from:

$$\sigma_{xy}^{2D;(2)} \equiv \sigma_z^{2D;(2)} = \frac{e^2}{h} \frac{1}{2} f, \quad (6)$$

where $f = \int_0^{2\pi} G_3(\theta) d\theta$, and we have recovered the units e^2/h . From the definition of G_3 in Eq. (5) one can see that θ plays exactly the same role as momentum and frequency. The integrand in Eq. (5) has a symmetric form if we view θ as a momentum component in an “extra dimension.” In the case of an insulator, f is a topological invariant which is equal to the second Chern number associated with the Bloch states of the 4+1D Hamiltonian $H[\mathbf{k}, \theta]$. For a TI, f will be odd, so one obtains a half-integral quantized transverse conductivity at the surface of a TI, when the surface is fully gapped [1].

For a doped TI, the Green’s functions have poles on the Fermi surface, so that f is in general not quantized. However, f is still invariant upon arbitrary smooth deformations of the Green’s function $G(\mathbf{k}, \theta, \omega)$ as long as the deformation vanishes at the Fermi surface. Making use of such topological invariance, we are able to integrate over frequency ω and obtain the following expression for f (see Supplementary Materials for the proof):

$$f = \frac{1}{32\pi^2} \int_{BZ} d^3\mathbf{k} \int_0^{2\pi} d\theta \text{Tr}(\mathcal{F}_{ab} \mathcal{F}_{cd}) \epsilon^{abcd}. \quad (7)$$

Here \mathcal{F}_{ab} is the Berry curvature associated with the bands that are filled, with $a, b = 1, 2, 3, 4$ labeling k_x, k_y, k_z, θ . More explicitly $\mathcal{F}_{ab}^{\alpha\beta} = \partial_a \mathcal{A}_b^{\alpha\beta} - \partial_b \mathcal{A}_a^{\alpha\beta} + i[\mathcal{A}_a, \mathcal{A}_b]^{\alpha\beta}$, $i\mathcal{A}_a^{\alpha\beta} = \langle \alpha\mathbf{k}\theta | \partial_a | \beta\mathbf{k}\theta \rangle$ with α, β running over filled bands. Formally, (7) looks the same as the second Chern number of the Berry phase gauge field that appears in the TI case.

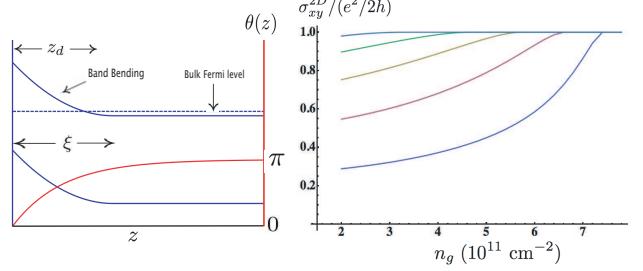


FIG. 2: Left: blue indicates schematically the band bending, displaying metallic bulk but gapped surface. Red indicates variation of θ from 0 to π . Right: numerical results for σ_{xy}^{2D} as a function of the top gate carrier density $n_g = CV_g/e$. The penetration depth of the T-breaking perturbation is chosen to be $\xi = 1$ nm, the depletion length is $z_d = n_g/n_b$, the bulk carrier density $n_b = 10^{16} \text{ cm}^{-3}$, and the Fermi level is chosen to be 18 meV from the conduction band bottom [26]. Starting from the bottom, the different curves correspond to $m_0 = 50, 100, 150, 200, 250$ meV, respectively. The gate carrier densities $n_g \sim 10^{11} \text{ cm}^{-2}$ are within experimentally accessible values.

However, for metallic systems there are different numbers of filled bands inside and outside each Fermi surface, so that the definition of \mathcal{F}_{ab} depends on the position of the Fermi surface and therefore f is *not* a second Chern number. For example, if there is a single Fermi surface, then $32\pi^2 f = \int_{FFS} \text{Tr} \mathcal{F}^{(1)} \wedge \mathcal{F}^{(1)} + \int_{BZ \setminus FFS} \text{Tr} \mathcal{F}^{(0)} \wedge \mathcal{F}^{(0)}$, where FFS denotes the filled Fermi sea, $\mathcal{F}^{(1)}$ is the Berry curvature associated with filled bands inside the Fermi surface, and $\mathcal{F}^{(0)}$ is the curvature associated with filled bands outside of the Fermi surface.

Since the second Chern form is a total derivative, f can be expressed, modulo an integer, in terms of integrals over the Fermi surfaces. We find that the fractional part of f is:

$$f \bmod 1 = \frac{1}{8\pi^2} \sum_i \int_{FS_i} \mathcal{L}_{CS}(\mathcal{A}^{P_i}), \quad (8)$$

where $\mathcal{L}_{CS}(\mathcal{A}) = \epsilon^{ijk} \text{Tr}[\mathcal{A}_i \partial_j \mathcal{A}_k + \frac{2i}{3} \mathcal{A}_i \mathcal{A}_j \mathcal{A}_k]$ is the Chern-Simons form. The sum is over the different Fermi surfaces, where FS_i labels the i th three-dimensional phase-space Fermi surface, and \mathcal{A}^{P_i} is the Berry connection associated with the partially filled bands that are crossing the i th Fermi surface, *i.e.* that have zero energy for $(\mathbf{k}, \theta) \in FS_i$. Eq. 8 is a consequence of a highly non-trivial cancellation of cross-terms associated with the non-Abelian CS forms, which is why only the partially filled bands participate. The proof of Eq. (7) and (8) is given in the Supplementary Materials.

Eq. (8) is an integral over the Berry connection involving only states at the Fermi surface. This is in direct analogy to Haldane’s result [19] that the fractional part of the intrinsic contribution to the anomalous Hall effect is due to the adiabatic phase acquired by quasiparticles

propagating on the Fermi surface. We see that inhomogeneities can also induce Berry phase contributions to the anomalous Hall effect, the fractional part of which depends only on states at the Fermi surface.

Note that in order for the above results to hold, we have assumed that θ varies slowly on the scale set by the mean free path. We must also assume that the Fermi surface vanishes near the surface of the material (see Figs. 1 and 2); otherwise, the surface will cause a sharp jump in the Fermi level and cannot be treated as a smooth change. If the Fermi level already lies in a gap at the surface, then the sharp jump in the chemical potential will not have consequences for the low energy physics.

Let us now apply our result to calculate the surface Hall conductivity of a realistic doped TI—doped Bi_2Se_3 . From the discrepancy between bulk transport measurements like Shubnikov-de Haas oscillations and surface measurements like ARPES, it has been noticed that the energy bands of Bi_2Se_3 (and Bi_2Te_3) can bend upwards near the surface, so that the Fermi level lies in the energy gap near the surface but in the conduction band in the bulk of the material (see Fig. 2) [26]. Such a situation can be further tuned using a top gate voltage. This can be described by our current approach since the gap near the surface effectively avoids the abrupt change in the band structure at the surface. The bulk of the system is TR invariant and can be described by the four-band effective model [2, 22] $H_0[\mathbf{k}] = \epsilon(\mathbf{k})\mathbb{I} + \sum_a d_a^{(0)}(\mathbf{k})\Gamma^a$ with Γ^a , $a = 0, 1, 2, 3$ the Dirac matrices and all the parameters $d_a^{(0)}(\mathbf{k})$ and $\epsilon(\mathbf{k})$ given in Ref. [2] (see also the Supplementary Materials).

We consider a T-breaking term induced by, *e.g.*, magnetic dopants deposited at the surface. Recently, angle-resolved photon emission (ARPES) experiments have observed a gap in the surface states of Mn doped Bi_2Te_3 [28], with the surface Fermi level lying in the gap. This system may provide an experimental realization of the surface TR symmetry breaking, although further verification of the nature of the surface gap is still needed. This can be described by adding the following surface term to the Hamiltonian:

$$H_1 = eV(z) + m_0 \sin[\theta(z)]\Gamma^3 - M_0(1 + \cos[\theta(z)])\Gamma^5, \quad (9)$$

where $eV(z) = -\frac{eCV_g}{4\epsilon\epsilon_0}z_d(1 - \frac{z}{z_d})^2$ is the potential induced by the top gate voltage, C is the capacitance per unit area of the dielectric separating the top gate and the surface of the TI, n_b is the bulk carrier density of the TI, V_g is the voltage applied at the top gate, $z_d = CV_g/en_b$ is the depeletion width induced by the top gate, and ϵ is the relative dielectric constant of the TI [29] (see Supplementary Materials). Note that charge neutrality requires z_d to be determined by the gate voltage, which reduced the number of free parameters in our calculation, allowing us to determine the Hall conductivity from realistic material

parameters.

We assume that the band bending near the surface is entirely induced by the top gate. $\theta(z) = \pi(1 - e^{-|z|/\xi})$ describes the surface TR symmetry breaking which decays exponentially versus the perpendicular distance z . The penetration depth ξ is set by the thickness of the layer of Mn dopants deposited at the surface; we take $\xi \approx 1\text{nm}$, assuming they penetrate several atomic layers into the surface. In a real system the T-breaking term may vary depending on details of the system. Here we take a simple T-breaking term. The Hamiltonian $H = H_0 + H_1$ can still be written in the Dirac form $H[\theta(z), \mathbf{k}] = (\epsilon(\mathbf{k}) - \mu + eV(z))\mathbb{I} + \sum_a d_a(\mathbf{k}, \theta)\Gamma^a$. All the z dependence can be absorbed into the parameter θ by defining $z(\theta) = -\xi \ln|1 - \theta/\pi|$. $d_a(\mathbf{k}, \theta) = d_a^{(0)}(\mathbf{k}, \theta) + \delta_{a,3}m_0 \sin[\theta] - \delta_{a,5}M_0(1 + \cos[\theta(z)])$. For this model Hamiltonian, $\sigma_{xy}^{2D;(1)}$ vanishes. f in Eq. (7) can be shown (see Supplementary Materials) to be given by

$$f = -\frac{3}{8\pi^2} \int_{\overline{FFS}} d^3k d\theta \epsilon_{abcd} \hat{d}_t \partial_x \hat{d}_a \partial_y \hat{d}_b \partial_z \hat{d}_c \partial_\theta \hat{d}_d, \quad (10)$$

where the integral is carried over the outside of electron Fermi pocket, denoted by \overline{FFS} and $\hat{d} = d/|d|$. As discussed earlier, θ can be viewed as the fourth momentum, playing the same role as the three-dimensional momenta $k_{x,y,z}$, and the three-dimensional phase space Fermi surface can be defined in the \mathbf{k}, θ space.

Numerical results of the surface Hall conductivity are shown in Fig. 2 as a function of the surface gate carrier density, $n_g = CV_g$, for different strengths of the gap induced by the magnetization, m_0 . Note our theory is only valid when the surface is gapped. The Hall conductivity saturates to the quantized value $e^2/2h$ in the limit that $z_d \approx n_g/n_b \gg \xi$. Physically this is because the T-breaking, and thus the nonzero Hall conductivity, only occurs in the range of $z \lesssim \xi$. For $\xi \ll z_d$ the system is insulating in the range of $z \lesssim \xi$, so that the surface Hall conductivity remains at the quantized value of TI surface. As expected, in the limit of low carrier density the Hall conductivity also approaches $e^2/2h$, which is dramatically different from an ordinary semiconductor in which the intrinsic Hall conductivity always vanishes in the limit of zero carrier density.

If observed, such a gate tunability of Hall conductivity in a *bulk* crystal provides a unique signature of doped TI compared to ordinary bulk semiconductors. We note that while disorder may add extrinsic contributions to the surface Hall conductance that we calculate here, these contributions vanish as the gate voltage is increased and the quantized $e^2/2h$ value is recovered. Our work provides quantitative estimates for achieving the quantized value, and by comparing with measurements, can be used as a way to estimate the strength of extrinsic contributions to the surface Hall conductance. Following the approach of Ref. [1] for topological insulators, our results can also

be extended to general dimensions. Such generalizations lead to a framework to study topological phenomena in Fermi liquids in generic dimensions, which we investigate in future work.

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SUPPLEMENTARY ONLINE MATERIAL

The purpose of these Supplementary Materials is to prove the following results (eqns. (7) and (8) of the main text):

$$\begin{aligned}
 f &\equiv -\frac{i\pi^2}{15} \epsilon^{\mu\nu\rho\sigma\tau} \int \frac{d^4 k d\omega}{(2\pi)^5} \text{Tr}[G \frac{\partial G^{-1}}{\partial q^\mu} G \frac{\partial G^{-1}}{\partial q^\nu} G \frac{\partial G^{-1}}{\partial q^\rho} G \frac{\partial G^{-1}}{\partial q^\sigma} G \frac{\partial G^{-1}}{\partial q^\tau}] \\
 &= \frac{1}{32\pi^2} \int_{BZ} d^3 \mathbf{k} \int_0^{2\pi} d\theta \text{Tr}(\mathcal{F}_{ab} \mathcal{F}_{cd}) \epsilon^{abcd},
 \end{aligned} \tag{11}$$

and

$$f \bmod 1 = \frac{1}{8\pi^2} \sum_i \int_{FS_i} \mathcal{L}_{CS}(\mathcal{A}^{P_i}). \tag{12}$$

The quantities \mathcal{A} and \mathcal{F} are defined in the text and will also be defined below. $q = (\omega, \mathbf{k})$ is a five-vector including the four-component spatial momentum \mathbf{k} and frequency ω , and $G = \sum_\alpha \frac{P_\alpha}{\omega - \xi_\alpha + i\delta \text{sgn}(\xi_\alpha)}$ is the non-interacting single-particle Green's function; P_α is a projector onto band α and $\xi_\alpha = \epsilon_\alpha - \mu$, where μ is the chemical potential. For a metal, f is not quantized; despite appearances, it is not a second Chern number because the definition of the matrix \mathcal{F} is such that its dimension changes at different points in momentum space, depending on the location of the Fermi surface(s).

The sections below are organized as follows. We begin by first manipulating the expression in terms of Green's functions into a more useful form. Next, we point out that even though f is not invariant under arbitrary deformations of the band structure, it is invariant under a certain class of deformations that we discuss. Following this, we prove some mathematical identities that the Berry connections of the Bloch bands must generally satisfy. Finally, after developing these ideas, we show how to use them to prove eqns. (11) and (12). We end with a discussion of the calculation of f in the simpler case of the Dirac models (Eq. (9) of the main text), which have additional symmetries.

PRELIMINARY MANIPULATIONS OF f

We have

$$\begin{aligned} G^{-1}(\mathbf{k}, \omega) &= \omega - H_{\mathbf{k}} + i\delta \text{sgn}(H_{\mathbf{k}}), \\ \partial_{\omega} G^{-1} &= 1 \\ \partial_i G^{-1} &= \partial_i H_{\mathbf{k}} \rightarrow \langle \alpha | \partial_i H_{\mathbf{k}} | \beta \rangle = \partial_i \xi_{\alpha}(\mathbf{k}) \delta_{\alpha\beta} + (\xi_{\beta} - \xi_{\alpha}) \langle \alpha | \partial_i | \beta \rangle \\ G(\mathbf{k}, \omega) &= \sum_{\alpha} \frac{P_{\alpha}}{\omega - \xi_{\alpha} + i\delta \text{sgn}(\xi_{\alpha})}, \end{aligned} \quad (13)$$

where $\partial_i = \frac{\partial}{\partial k_i}$ is a derivative with respect to a momentum coordinate. Inserting a complete set of states for each \mathbf{k} , we have:

$$f = -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \epsilon^{ijkl} \int d^4 k d\omega \sum_{\alpha\beta\gamma\delta} A_i^{\alpha\beta} A_j^{\beta\gamma} A_k^{\gamma\delta} A_l^{\delta\alpha} d_{\alpha}^2 d_{\beta} d_{\gamma} d_{\delta}, \quad (14)$$

where we have set $A_i^{\alpha\beta} = \langle \alpha | \partial_i G^{-1} | \beta \rangle$ and $d_{\alpha}^{-1} = \omega - \xi_{\alpha} + i\delta \text{sgn}(\xi_{\alpha})$.

Now observe that the above sum vanishes whenever at least any three of $\alpha, \beta, \gamma, \delta$ are equal. For example if $\beta = \gamma = \delta$, then the summand is $d_{\alpha}^2 d_{\beta}^3 A_i^{\alpha\beta} A_j^{\beta\beta} A_k^{\beta\beta} A_l^{\beta\alpha}$, which vanishes upon contraction with the epsilon tensor. Similarly, if $\alpha = \beta = \gamma$, the summand is $d_{\alpha}^4 d_{\delta} A_i^{\alpha\alpha} A_j^{\alpha\alpha} A_k^{\alpha\delta} A_l^{\delta\alpha}$, which also vanishes upon contraction with the epsilon tensor.

Thus we are left with 3 types of terms:

$$f = -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \epsilon^{ijkl} \int d^4 k d\omega \left(\sum'_{\alpha\beta\gamma\delta} + \sum''_{\alpha\beta\gamma\delta} + \sum'''_{\alpha\beta\gamma\delta} \right) A_i^{\alpha\beta} A_j^{\beta\gamma} A_k^{\gamma\delta} A_l^{\delta\alpha} d_{\alpha}^2 d_{\beta} d_{\gamma} d_{\delta} \quad (15)$$

In $\sum'_{\alpha\beta\gamma\delta}$, the sum is over states $(\alpha, \beta, \gamma, \delta)$ that are all different. In $\sum''_{\alpha\beta\gamma\delta}$, the sum is over states where exactly two of the indices are equal and the others are all different. Finally, $\sum'''_{\alpha\beta\gamma\delta}$ is over states where two pairs of indices take the same value (e.g. $\alpha = \beta$ and $\gamma = \delta$ but $\alpha \neq \gamma$).

Let us first show that the last sum gives zero contribution. Its contribution is proportional to:

$$\int d^4 k d\omega \sum_{\alpha\beta\gamma\delta} (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \epsilon^{ijkl} A_i^{\alpha\beta} A_j^{\beta\gamma} A_k^{\gamma\delta} A_l^{\delta\alpha} d_{\alpha}^2 d_{\beta} d_{\gamma} d_{\delta} \quad (16)$$

It is easy to see that the second term vanishes because of the epsilon tensor, and that the first and third terms cancel each other after indices are relabelled (to see this, note that $\epsilon^{lijk} = -\epsilon^{ijkl}$, since cyclic permutations have odd signature in even dimensions).

Therefore, we see that the third sum in (15) vanishes. Now consider the second sum in (15), which we will call B :

$$B \equiv -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \sum''_{\alpha\beta\gamma\delta} \epsilon^{ijkl} \int d^4 k d\omega A_i^{\alpha\beta} A_j^{\beta\gamma} A_k^{\gamma\delta} A_l^{\delta\alpha} d_{\alpha}^2 d_{\beta} d_{\gamma} d_{\delta} \quad (17)$$

Recall that $\sum''_{\alpha\beta\gamma\delta}$ is a sum over states where exactly two of the indices are equal and the rest are all different. There are exactly 6 ways this can happen; let us write each one out:

$$B = B_{\alpha=\beta} + B_{\alpha=\gamma} + B_{\alpha=\delta} + B_{\beta=\gamma} + B_{\beta=\delta} + B_{\gamma=\delta}, \quad (18)$$

where the subscripts indicate which terms in the sum are to be set equal to each other. We find that $B_{\alpha=\beta} + B_{\alpha=\delta} = 0$. We also find

$$\begin{aligned} B_{\alpha=\gamma} + B_{\beta=\delta} &= -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \epsilon^{ijkl} \sum'_{\alpha\beta\delta} \int d^4k d\omega A_i^{\alpha\beta} A_j^{\beta\alpha} A_k^{\alpha\delta} A_l^{\delta\alpha} d_\alpha^2 d_\beta d_\delta (d_\alpha - d_\beta). \\ B_{\beta=\gamma} + B_{\gamma=\delta} &= -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \epsilon^{ijkl} \sum'_{\alpha\beta\gamma} \int d^4k d\omega (A_i^{\alpha\beta} A_j^{\beta\beta} A_k^{\beta\gamma} A_l^{\gamma\alpha} - c.c.) d_\alpha^2 d_\beta^2 d_\gamma \end{aligned} \quad (19)$$

$\sum'_{\alpha\beta\gamma}$ indicates a sum over states where α, β, γ are all different. *c.c.* denotes complex conjugation. Note that $(A_i^{\alpha\beta})^* = -A_i^{\beta\alpha}$ if $\alpha \neq \beta$ while $A_i^{\alpha\alpha} = \partial_i \xi_\alpha$ is real.

Therefore, we see that f is given by the following sum of three terms:

$$\begin{aligned} f &= -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \int d^4k (x + y + z) \\ x(\mathbf{k}) &= \epsilon^{ijkl} \sum'_{\alpha\beta\gamma\delta} \xi_{\alpha\beta} \xi_{\beta\gamma} \xi_{\gamma\delta} \xi_{\delta\alpha} \mathcal{A}_i^{\alpha\beta} \mathcal{A}_j^{\beta\gamma} \mathcal{A}_k^{\gamma\delta} \mathcal{A}_l^{\delta\alpha} \int d\omega d_\alpha^2 d_\beta d_\gamma d_\delta \\ y(\mathbf{k}) &= \epsilon^{ijkl} \sum'_{\alpha\beta\delta} \xi_{\alpha\beta}^2 \xi_{\alpha\delta}^2 \mathcal{A}_i^{\alpha\beta} \mathcal{A}_j^{\beta\alpha} \mathcal{A}_k^{\alpha\delta} \mathcal{A}_l^{\delta\alpha} \int d\omega d_\alpha^2 d_\beta d_\delta (d_\alpha - d_\beta). \\ z(\mathbf{k}) &= -i\epsilon^{ijkl} \sum'_{\alpha\beta\gamma} \partial_i \xi_\beta \xi_{\beta\alpha} \xi_{\gamma\beta} \xi_{\alpha\gamma} (\mathcal{A}_j^{\alpha\beta} \mathcal{A}_k^{\beta\gamma} \mathcal{A}_l^{\gamma\alpha} + \mathcal{A}_j^{\alpha\gamma} \mathcal{A}_k^{\gamma\beta} \mathcal{A}_l^{\beta\alpha}) \int d\omega d_\alpha^2 d_\beta^2 d_\gamma \end{aligned} \quad (20)$$

where we have set $i\mathcal{A}_i^{\alpha\beta} = \langle \alpha; \mathbf{k} | \partial_i | \beta; \mathbf{k} \rangle$ and $\xi_{\alpha\beta} \equiv \xi_\alpha - \xi_\beta$. The important point to note here is that $x(\mathbf{k})$ and $y(\mathbf{k})$ do not depend on the slope of the dispersion, $\partial_i \xi_\alpha$, while $z(\mathbf{k})$ does.

Note that in the sum in $z(\mathbf{k})$, all three bands α, β and γ must have different energies. Consequently, for a special class of models such as the Dirac-type models, which have only two bands with distinct energies (each of which generically has a degeneracy), $z(\mathbf{k})$ must be zero. In these cases, it is easy to show that the integrand in the remaining terms are independent of the energy spectrum and are proportional to $\text{Tr} \mathcal{F} \wedge \mathcal{F}$. Thus a direct and explicit evaluation of $x(\mathbf{k}) + y(\mathbf{k})$ reveals eq. (F1).

Topological invariance of f upon smooth deformations of G

For general band structures with three or more distinct energy levels, the proof of eq. (11) is more nontrivial and it is essential to exploit the topological invariance of f to deformations that preserve the band structure near the Fermi surface. Under a smooth deformation of G to $G + \delta G$, the variation of f is given by

$$\delta f = \frac{i\pi^2}{15} \epsilon^{\mu\nu\rho\sigma\tau} \int \frac{d^4k d\omega}{(2\pi)^5} \partial_\mu \text{Tr} [(G^{-1} \delta G) (\partial_\nu G^{-1} G) (\partial_\nu G^{-1} G) (\partial_\nu G^{-1} G) (\partial_\nu G^{-1} G)]. \quad (21)$$

Note that a deformation of the band structure that changes the location of the Fermi surface is not a smooth deformation, because it can move the poles of G from the upper half plane to the lower half plane (or vice versa), and these are not small changes. Therefore, a small deformation of the band structure corresponds to a small deformation of G provided that it is away from the Fermi surface. Thus we can only deform the band structure if we keep a small window near the Fermi surface unchanged. Observe that since the integrand in (21) is a total derivative, it will vanish if δG vanishes at the boundaries of the integral. Therefore, we can deform an arbitrary band structure (Fig. 3a) into a flat band dispersion (Fig. 3b), where the band structure is unchanged in a small window near the Fermi surface. We may take the limit that the size of the window goes to zero at the end of the calculation.

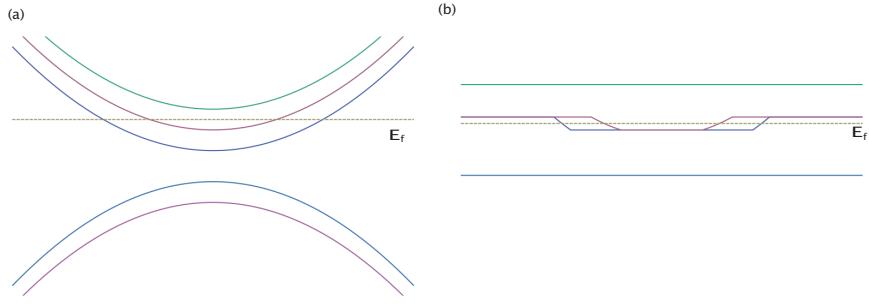


FIG. 3: (a) Cross-section of a generic band structure, with the Fermi level lying within a band. (b) Deformation of band structure in such a way that f is left invariant. The filled and empty bands are deformed to a flat band, while the partially filled bands are deformed to flat bands everywhere except a small window near the Fermi surface, where they are left unchanged.

Identities

For the proof of eqn. (11) and (12), here we will prove the following identity:

$$\epsilon^{ijk} \sum_{P,\gamma} \int_{FS} \mathcal{A}_i^{(M);P\gamma} \mathcal{F}_{jk}^{(M);\gamma P} = 0. \quad (22)$$

FS stands for an arbitrary 3D Fermi surface in the 4D Brillouin zone. $\mathcal{F}^{(M)}$ is the curvature associated with M bands, including m bands below the Fermi surface labeled by γ and $M - m$ bands crossing the Fermi surface labeled by P . Our proof will require us to be able to set $\xi_P(\mathbf{k}) > \xi_\gamma(\mathbf{k})$ for all \mathbf{k} , so (22) is true only for those bands for which this is possible.

First we observe that for an insulator,

$$f = \frac{1}{32\pi^2} \int_{BZ} Tr \mathcal{F} \wedge \mathcal{F}, \quad (23)$$

where \mathcal{F} is the field strength of the Berry connection associated with the filled bands. This formula is easy to prove in the case that the bands are all flat, with the empty/filled bands having energy ξ_E or ξ_F , respectively [1]. For a general band structure, it is argued that f is invariant under deformations of the band structure, and so its value is given by deforming the energy dispersions to the flat band model. This means that the terms in (20) that depend on energy must vanish, imposing various constraints on the properties of the Berry connections. (22) is one of these constraints; here we will derive it, along with some others as well.

First we consider a band structure with flat energy dispersions ξ_E , ξ_P , and ξ_F , each of which may be multiply degenerate. When ξ_E and ξ_P are empty, it is easy to show that

$$\begin{aligned} x(\mathbf{k}) + y(\mathbf{k}) = & -6 * 2\pi i (A_{EFEF} + A_{PFPF} + A_{PFEF} + A_{EFFP}) \\ & + 8\pi i \sum_{n=2}^{\infty} (-\xi_{EP}/\xi_{FE})^n (A_{PEPF} - A_{PEFE} - A_{PFEF}) \end{aligned} \quad (24)$$

We have set

$$A_{ABCD} = \epsilon_{ijkl} \sum_{(\alpha,\beta,\gamma,\delta) \in (A,B,C,D)} \mathcal{A}_i^{\alpha\beta} \mathcal{A}_j^{\beta\gamma} \mathcal{A}_k^{\gamma\delta} \mathcal{A}_l^{\delta\alpha}, \quad (25)$$

where the indices A, B, C, D can refer to P, E , or F . When the bands are all flat, $z(\mathbf{k}) = 0$, so $f = -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} \int d^4k (x + y)$. Since the second terms (whose coefficients depend on the energies) must vanish, it follows that

$$\int d^4k (A_{PEPF} - A_{PEFE} - A_{PFEF}) = 0. \quad (26)$$

Now consider a general band structure for an arbitrary insulator that has M filled bands. We know that we can deform the bands however we like without changing f , as long as no band crosses the Fermi level during the

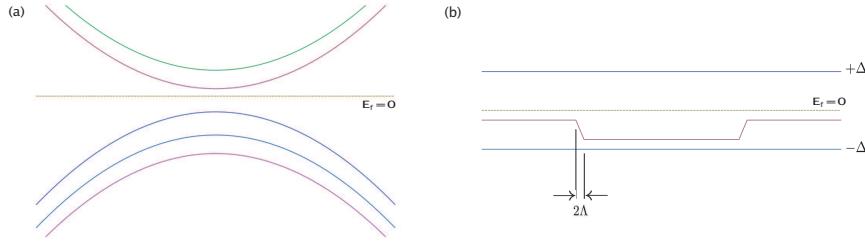


FIG. 4: (a) Cross-section of a generic band structure with M filled bands. (b) Deformed band structure: the empty bands are deformed to a flat band with energy Δ , m filled bands are deformed to flat bands with energy $-\Delta$, and $M - m$ filled bands are deformed so that the energy is flat everywhere except in a small window of width 2Λ where it varies linearly, as discussed in the main text.

deformation. Let us deform them in the following way: consider a band structure where there are bands with energy ξ_E that are empty, m bands with energy ξ_F that are filled, and $M - m$ bands with energy ξ_P that are filled. ξ_E and ξ_F will be flat bands, with energy $\pm\Delta$, respectively. ξ_P will be flat everywhere except a small region in the BZ, where it varies linearly (See Fig. 4). More specifically, pick a boundaryless 3-manifold, called FS , and suppose that ξ_P varies linearly with distance from FS in some shell of thickness 2Λ around FS . In this case, $Z = \int_{BZ} d^4k z(\mathbf{k})$ is given by

$$\begin{aligned}
Z &= -i\epsilon^{ijkl} \sum_P \sum_{\alpha\gamma} \int_{FS \pm \Lambda} d^4k \partial_i \xi_P \xi_{P\alpha} \xi_{\gamma P} \xi_{\alpha\gamma} (\mathcal{A}_j^{\alpha P} \mathcal{A}_k^{P\gamma} \mathcal{A}_l^{\gamma\alpha} + \mathcal{A}_j^{\alpha\gamma} \mathcal{A}_k^{\gamma P} \mathcal{A}_l^{P\alpha}) \int d\omega d_\alpha^2 d_P^2 d_\gamma, \\
&= -i\epsilon^{ijkl} \sum_P \int_{FS \pm \Lambda} d^4k d\omega \xi_{FP} \xi_{EF} \xi_{PE} \partial_i \xi_P d_P^2 d_E d_F (d_E - d_F) \sum_{\beta \in E, \gamma \in F} (\mathcal{A}_j^{\alpha P} \mathcal{A}_k^{P\gamma} \mathcal{A}_l^{\gamma\alpha} + \mathcal{A}_j^{\alpha\gamma} \mathcal{A}_k^{\gamma P} \mathcal{A}_l^{P\alpha}) \\
&= \epsilon^{ijkl} \sum_P \int_{FS \pm \Lambda} d^4k d\omega \xi_{FP} \xi_{EF} \xi_{PE} \partial_i \xi_P d_P^2 d_E d_F (d_E - d_F) \frac{1}{2} \sum_{\gamma \in F} (\mathcal{A}_j^{P\gamma} \mathcal{F}_{kl}^{\gamma P} + \mathcal{A}_j^{\gamma P} \mathcal{F}_{kl}^{P\gamma}) \\
&= \int_{FS \pm \Lambda} d^4k d\omega V^i \partial_i \xi_P \xi_{FP} \xi_{EF} \xi_{PE} d_P^2 d_E d_F (d_E - d_F) \\
&= 2\pi i \int_{FS \pm \Lambda} d^4k V^i \partial_i \xi_P \xi_{PF} \xi_{FE} \xi_{EP} \left[\frac{1}{\xi_{FP}^2 \xi_{FE}^2} + \frac{1}{\xi_{EP}^2 \xi_{EF}^2} - \frac{1}{\xi_{PE}^2 \xi_{PF}^2} - \frac{2}{\xi_{PE}^3 \xi_{PF}} \right], \tag{27}
\end{aligned}$$

where we have set $V^i(\mathbf{k}) = \frac{1}{2} \sum_P \sum_{\gamma \in F} (\mathcal{A}_j^{P\gamma} \mathcal{F}_{kl}^{\gamma P} + \mathcal{A}_j^{\gamma P} \mathcal{F}_{kl}^{P\gamma})$. For the sake of being explicit, we set the energy dispersions to be:

$$\xi_E = -\xi_F = \Delta,$$

$$\xi_P(\mathbf{k}) = \begin{cases} \frac{\Delta}{4\Lambda} \kappa - \Delta/2 & \text{if } \mathbf{k} \in (FS \pm \Lambda) \\ -\Delta/4 & \text{if } \mathbf{k} \in (BZ \setminus (FFS + \Lambda)) \\ -3\Delta/4 & \text{if } \mathbf{k} \in (FFS - \Lambda) \end{cases} \tag{28}$$

Here we have set κ to be the distance in the direction \hat{n} normal to FS .

$$\begin{aligned}
\xi_{PF} &= \Delta(1 + \xi_P/\Delta) = \Delta(1/2 + \kappa/4\Lambda) \\
\xi_{EP} &= \Delta(1 - \xi_P/\Delta) = \Delta(3/2 - \kappa/4\Lambda) \tag{29}
\end{aligned}$$

$$Z = 2\pi i \frac{\Delta}{4\Lambda} \int_{FS \pm \Lambda} d^4k V^i \xi_{PF} \xi_{FE} \xi_{EP} \left[\frac{1}{\xi_{FP}^2 \xi_{FE}^2} + \frac{1}{\xi_{EP}^2 \xi_{EF}^2} - \frac{1}{\xi_{PE}^2 \xi_{PF}^2} - \frac{2}{\xi_{PE}^3 \xi_{PF}} \right]. \tag{30}$$

After some simplification, this becomes

$$\begin{aligned}
Z &= -\pi i \int_{-1}^1 d\kappa' \int_{FS} d^3k_{||} V^i (\Lambda \kappa', \mathbf{k}_{||}) \left(\frac{1}{2} + \frac{\kappa'}{4} \right) \left(\frac{3}{2} - \frac{\kappa'}{4} \right) \times \\
&\quad \left[\frac{1}{4(1/2 + \kappa'/4)^2} + \frac{1}{4(3/2 - \kappa'/4)^2} - \frac{1}{(1/2 + \kappa'/4)^2 (3/2 - \kappa'/4)^2} + \frac{2}{(3/2 - \kappa'/4)^3 (1/2 + \kappa'/4)} \right], \tag{31}
\end{aligned}$$

where we have made a change of variables $\kappa' = \kappa/\Lambda$. Thus, it is clear that

$$\lim_{\substack{\Delta, \Lambda \rightarrow 0 \\ \Delta/\Lambda \text{ fixed}}} Z \propto \int_{FS} V \cdot \hat{n} \quad (32)$$

Now observe that

$$f = \frac{1}{32\pi^2} \int d^4k Tr F \wedge F + \delta f^{out} + \delta f^{in}, \quad (33)$$

where δf^{out} arises from the contribution of integrals outside of $FS \pm \Lambda$, while δf^{in} arises from contributions of integrals over $FS \pm \Lambda$:

$$\begin{aligned} \delta f^{out} &= \frac{-i\pi^2}{3} \frac{1}{(2\pi)^5} 8\pi i \sum_{n=2}^{\infty} (-\xi_{EP}/\xi_{FE})^n \left(\int_{BZ \setminus (FFS + \Lambda)} + \int_{FFS - \Lambda} \right) d^4k [(A_{PEPF} - A_{PEFE} - A_{PFEF})] \\ \delta f^{in} &= \frac{-i\pi^2}{3} \frac{1}{(2\pi)^5} 8\pi i \sum_{n=2}^{\infty} (-1/\xi_{FE})^n \int_{FS \pm \Lambda} d^4k \xi_{EP}^n(\mathbf{k}) [A_{PEPF} - A_{PEFE} - A_{PFEF}] + Z \end{aligned} \quad (34)$$

For any choice of Δ , it must be the case that

$$\delta f^{out} + \delta f^{in} = 0, \quad (35)$$

because f is actually given by the first term of (33). First observe that

$$\lim_{\substack{\Delta, \Lambda \rightarrow 0 \\ \Delta/\Lambda \text{ fixed}}} \delta f^{in} = \lim_{\substack{\Delta, \Lambda \rightarrow 0 \\ \Delta/\Lambda \text{ fixed}}} Z. \quad (36)$$

This is because in that limit, it is clear that $\sum_{n=2}^{\infty} \int_{FS \pm \Lambda} d^4k [(\xi_{EP}(\mathbf{k})/\xi_{EF})^n (A_{PEPF} - A_{PEFE} - A_{PFEF})] \rightarrow 0$, because the integrand is finite while the integration region becomes vanishingly small. Furthermore,

$$\lim_{\substack{\Delta, \Lambda \rightarrow 0 \\ \Delta/\Lambda \text{ fixed}}} \delta f^{out} \propto \sum_{n=2}^{\infty} (-\xi_{EP}/\xi_{FE})^n \int d^4k [(A_{PEPF} - A_{PEFE} - A_{PFEF})] = 0. \quad (37)$$

The last equality above follows from eqn. (26). From the above equations, it follows that

$$\lim_{\substack{\Delta, \Lambda \rightarrow 0 \\ \Delta/\Lambda \text{ fixed}}} Z \propto \int_{FS} V \cdot \hat{n} = 0 \quad (38)$$

Now observe that

$$\int_{FS} V \cdot \hat{n} \propto \epsilon^{ijk} \sum_{P,\gamma} \int_{FS} \mathcal{A}_i^{(M);P\gamma} \mathcal{F}_{jk}^{(M);\gamma P} = 0, \quad (39)$$

which proves the identity (22).

Proof of Eqn. (11)

Armed with the identity (22), here we will prove eqn. (11) by deforming an arbitrary band structure – in the case where the chemical potential lies inside a band – in such a way that keeps f unchanged while making it amenable to calculation.

Consider the following deformation of the band structure, which keeps f unchanged because it does not deform the partially filled bands in a window near the Fermi surface (see Fig. 5). As in the previous section, we will use the variable κ to denote the distance from the Fermi surface, and k_{\parallel} to be the directions parallel to the Fermi surface. Choose some small energy Δ near zero so that there exists Λ_1 and Λ_2 where $\xi_P(\kappa = \Lambda_1) = \Delta$ and $\xi_P(\kappa = \Lambda_2) = -\Delta$. Deform the empty and filled bands to have a flat dispersion, with energy $\pm\Delta$. Then, deform the partially filled band for $\kappa \geq \Lambda_1$ to have a flat dispersion with energy Δ . Finally deform the partially filled band for $\kappa \leq \Lambda_2$ to have a flat

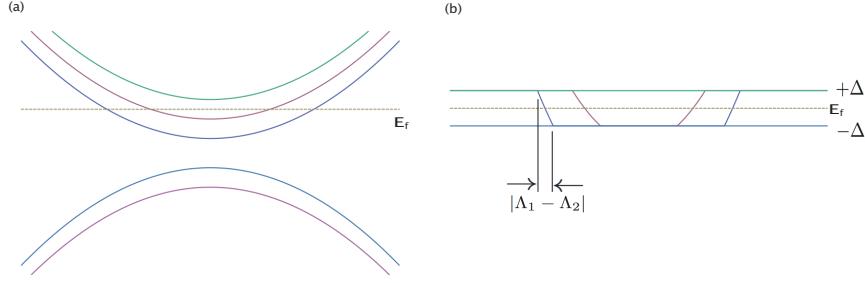


FIG. 5: (a) Cross section of generic band structure with partially filled bands. (b) Deformed band structure. The bands are deformed to flat bands with energy $\pm\Delta$ relative to the Fermi level everywhere outside of a small window near the Fermi surface. Inside the small window near the Fermi surface, the bands are unchanged. The limit $\Delta \rightarrow 0$ is taken at the end of the calculation.

dispersion with energy $-\Delta$. For $\Lambda_2 \leq \kappa \leq \Lambda_1$, the dispersion of the partially filled band is unchanged. The region where $\Lambda_2 \leq \kappa \leq \Lambda_1$ will be denoted as $FS \pm \Lambda$.

Now we can split up the integrals over momentum space into a sum of integrals:

$$f = -\frac{i\pi^2}{3} \frac{1}{(2\pi)^5} [(X_{out} + Y_{out} + Z_{out}) + (X_{in} + Y_{in} + Z_{in})], \quad (40)$$

where $X_{out} = \int_{BZ \setminus (FS \pm \Lambda)} d^4k x(\mathbf{k})$, $X_{in} = \int_{FS \pm \Lambda} d^4k x(\mathbf{k})$, and analogously for Y and Z . $Z_{out} = 0$ because it depends on $\partial \xi_\alpha$, and

$$-\frac{\pi^2}{3} \frac{1}{(2\pi)^5} (X_{out} + Y_{out} + Z_{out}) = \frac{1}{32\pi^2} \int_{\kappa > \Lambda_1} d^4k \epsilon^{ijkl} \text{Tr}[\mathcal{F}_{ij}^{(M)} \mathcal{F}_{kl}^{(M)}] + \frac{1}{32\pi^2} \int_{\kappa < \Lambda_2} d^4k \epsilon^{ijkl} \text{Tr}[\mathcal{F}_{ij}^{(M+P)} \mathcal{F}_{kl}^{(M+P)}], \quad (41)$$

where $\mathcal{F}^{(M)}$ is the Berry curvature for the M filled bands outside of FS , while $\mathcal{F}^{(M+P)}$ is the Berry curvature for the M filled bands and the P partially filled bands whose Fermi surface FS we are considering.

Observe that in the limit $\Delta \rightarrow 0$, $X_{in} + Y_{in} \rightarrow 0$ because the size of the region of integration goes to zero while the integrand stays finite. In the following, we will show that

$$\lim_{\Delta \rightarrow 0} Z \propto \epsilon^{ijk} \sum_{P,\gamma} \int_{FS} \mathcal{A}_i^{(M);P\gamma} \mathcal{F}_{jk}^{(M);\gamma P} = 0, \quad (42)$$

which will show that in the case of a single Fermi surface,

$$f = \frac{1}{32\pi^2} \int_{BZ \setminus FFS} d^4k \epsilon^{ijkl} \text{Tr}[\mathcal{F}_{ij}^{(M)} \mathcal{F}_{kl}^{(M)}] + \frac{1}{32\pi^2} \int_{FFS} d^4k \epsilon^{ijkl} \text{Tr}[\mathcal{F}_{ij}^{(M+P)} \mathcal{F}_{kl}^{(M+P)}]. \quad (43)$$

The generalization to multiple non-intersecting Fermi surfaces is straightforward.

Now consider Z :

$$\begin{aligned} Z &= -i\epsilon^{ijkl} \sum_P \sum_{\alpha\gamma} \int_{FS \pm \Lambda} d^4k \partial_i \xi_P \xi_{P\alpha} \xi_{\gamma P} \xi_{\alpha\gamma} (\mathcal{A}_j^{\alpha P} \mathcal{A}_k^{P\gamma} \mathcal{A}_l^{\gamma\alpha} + \mathcal{A}_j^{\alpha\gamma} \mathcal{A}_k^{\gamma P} \mathcal{A}_l^{P\alpha}) \int d\omega d_\alpha^2 d_P^2 d_\gamma, \\ &= -i\epsilon^{ijkl} \sum_P \int_{FS \pm \Lambda} d^4k d\omega \xi_{FP} \xi_{EF} \xi_{PE} \partial_i \xi_P d_P^2 d_E d_F (d_E - d_F) \sum_{\beta \in E, \gamma \in F} (\mathcal{A}_j^{\alpha P} \mathcal{A}_k^{P\gamma} \mathcal{A}_l^{\gamma\alpha} + \mathcal{A}_j^{\alpha\gamma} \mathcal{A}_k^{\gamma P} \mathcal{A}_l^{P\alpha}) \\ &= \epsilon^{ijkl} \sum_P \int_{FS \pm \Lambda} d^4k d\omega \xi_{FP} \xi_{EF} \xi_{PE} \partial_i \xi_P d_P^2 d_E d_F (d_E - d_F) \frac{1}{2} \sum_{\gamma \in F} (\mathcal{A}_j^{P\gamma} \mathcal{F}_{kl}^{\gamma P} + \mathcal{A}_j^{\gamma P} \mathcal{F}_{kl}^{P\gamma}) \\ &= \int_{FS \pm \Lambda} d^4k d\omega V^i \partial_i \xi_P \xi_{FP} \xi_{EF} \xi_{PE} d_P^2 d_E d_F (d_E - d_F) \\ &= 2\pi i \int_{FS \pm \Lambda} d^4k V^i \partial_i \xi_P \xi_{PF} \xi_{FE} \xi_{EP} \left[\frac{1}{\xi_{FP}^2 \xi_{FE}^2} + \frac{1}{\xi_{EP}^2 \xi_{EF}^2} - \frac{1}{\xi_{PE}^2 \xi_{PF}^2} - \frac{2}{\xi_{PE} \xi_{PF}^3} \right. \\ &\quad \left. 2n_P \left(\frac{1}{\xi_{PE} \xi_{PF}^3} - \frac{1}{\xi_{PE}^3 \xi_{PF}} \right) \right], \end{aligned} \quad (44)$$

We have:

$$\begin{aligned}\xi_{PF} &= \Delta(1 + X) \\ \xi_{EF} &= 2\Delta \\ \xi_{EP} &= \Delta(1 - X), \\ X &= \xi_P/\Delta.\end{aligned}\tag{45}$$

Thus

$$Z \propto \frac{1}{\Delta} \int_{FS \pm \Lambda} d^4 k V \cdot \partial \xi_P I(\mathbf{k}, \Lambda_1),\tag{46}$$

where

$$\begin{aligned}I(\mathbf{k}, \Lambda_1) &= (1 + X)(1 - X) \left[\frac{1}{4(1 + X)^2} + \frac{1}{4(1 - X)^2} - \frac{1}{(1 - X)^2(1 + X)^2} + \frac{2}{(1 - X)(1 + X)^3} + 2n_P \left(\frac{1}{(1 - X)^3(1 + X)} \right. \right. \\ &\quad \left. \left. - \frac{1}{(1 - X)(1 + X)^3} \right) \right].\end{aligned}\tag{47}$$

Simplifying:

$$I(\mathbf{k}, \Lambda_1) = \begin{cases} \frac{(1-X)(X+3)}{2(1+X)^2} & \text{if } X(\mathbf{k}) > 0 \\ \frac{(1+X)(3-X)}{2(1-X)^2} & \text{if } X(\mathbf{k}) \leq 0 \end{cases}\tag{48}$$

In the limit $\Delta \rightarrow 0$, which by definition also takes $\Lambda_i \rightarrow 0$ while keeping Δ/Λ_i fixed, we see that the size of the integration region is proportional to $\Lambda_1 - \Lambda_2$, while $I(\mathbf{k}, \Lambda_1)$ is non-singular. It follows that

$$\lim_{\Delta \rightarrow 0} Z \propto \int_{FS} V \cdot \partial \xi_P \propto \int_{FS} V \cdot \hat{n},\tag{49}$$

where the latter proportionality follows because ξ_P has non-zero slope at the Fermi surface only in the direction normal to the Fermi surface. From the definition of V , (42) follows.

PROOF OF EQN. (12)

In the last section, we proved the highly non-trivial relation

$$f = \frac{1}{32\pi^2} \int d^4 \mathbf{k} \text{Tr}(\mathcal{F}_{ab} \mathcal{F}_{cd}) \epsilon^{abcd}.\tag{50}$$

The dependence on the chemical potential is implicit in the definition of the field strength $\mathcal{F}(\mathbf{k})$. $\mathcal{F}(\mathbf{k})$ is defined to be the field strength of the Berry connection for the bands that are filled at the point \mathbf{k} in the four-dimensional Brillouin Zone. Depending on the location of the Fermi surface(s), the number of filled bands will be different at different \mathbf{k} -points. This is not the typical formula for a second Chern invariant.

Here we prove a more mathematical result:

$$f \bmod 1 = \frac{1}{8\pi^2} \sum_i \int_{FS_i} \mathcal{L}_{CS}(\mathcal{A}^{P_i}),\tag{51}$$

where $\mathcal{A}^{(P_i)}$ is the Berry connection involving only the partially filled bands that are part of the i th Fermi surface FS_i .

In order to prove this, let us first concentrate on the case of a single Fermi surface. We may rewrite f as

$$f = \frac{1}{32\pi^2} \int_{BZ \setminus FFS} \text{Tr}(\mathcal{F}_{ab}^{(0)} \mathcal{F}_{cd}^{(0)}) \epsilon^{abcd} + \frac{1}{32\pi^2} \int_{FFS} \text{Tr}(\mathcal{F}_{ab}^{(1)} \mathcal{F}_{cd}^{(1)}) \epsilon^{abcd},\tag{52}$$

where FFS indicates the filled Fermi sea, *ie* the region in momentum space inside the Fermi surface, while $BZ \setminus FFS$ indicates the region outside of the filled Fermi sea. $\mathcal{F}^{(0)}$ involves the completely filled bands, while $\mathcal{F}^{(1)}$ involves the completely filled bands and the partially filled bands.

Now observe that $F_{ab}F_{cd}\epsilon^{abcd}$ is locally a total derivative:

$$F_{ab}F_{cd}\epsilon^{abcd} = 4\partial_a(A_b\partial_cA_d + \frac{2i}{3}A_bA_cA_d)\epsilon^{abcd}, \quad (53)$$

which implies:

$$f \bmod 1 = \frac{1}{8\pi^2} \int_{FS} [\mathcal{L}_{CS}(\mathcal{A}^{(1)}) - \mathcal{L}^{CS}(\mathcal{A}^{(0)})], \quad (54)$$

where $\mathcal{A}^{(0)}$ is the non-Abelian Berry connection for the completely filled bands, $\mathcal{A}^{(1)}$ is the non-Abelian Berry connection for the completely and partially filled bands, and $\mathcal{L}^{CS}(A) = \epsilon^{\mu\nu\lambda}\text{Tr}[A_\mu\partial_\nu A_\lambda + \frac{2i}{3}A_\mu A_\nu A_\lambda]$ is the Chern-Simons form. Since the Chern-Simons form is non-linear, this subtraction has a cross-term:

$$f \bmod 1 = \frac{1}{8\pi^2} \int_{FS} [\mathcal{L}_{CS}(\mathcal{A}^{(P)}) + \epsilon^{ijk} \sum_{\gamma \in F, P} \mathcal{A}_i^{P\gamma} \mathcal{F}_{jk}^{(1); \gamma P}]. \quad (55)$$

The second term vanishes by Eq. (22), so that we obtain

$$f \bmod 1 = \frac{1}{8\pi^2} \int_{FS} \mathcal{L}_{CS}(\mathcal{A}^{(P)}). \quad (56)$$

The generalization to multiple Fermi surfaces is straightforward and yields (51).

f FOR DIRAC -TYPE MODELS

Consider the Hamiltonian

$$H(\mathbf{k}) = \epsilon(\mathbf{k})\mathbb{I} + d_a\Gamma^a, \quad (57)$$

where Γ^a for $a = 1, \dots, 5$ are the 4×4 Γ matrices; their relation to the physical properties of Bi_2Se_3 are described in [2]. The eigenvalues of this Hamiltonian are $\xi_{\pm}(\mathbf{k}) = \epsilon(\mathbf{k}) \pm |d(\mathbf{k})|$; each band is doubly degenerate. $P_{\pm} = \frac{1}{2}(1 \pm \hat{d} \cdot \Gamma)$ projects onto the bands with energies ξ_{\pm} . The Green's function is:

$$\begin{aligned} G(\mathbf{k}, \omega) &= \frac{P_+}{\omega - \xi_+ + i\delta\text{sgn}(\xi_+)} + \frac{P_-}{\omega - \xi_- + i\delta\text{sgn}(\xi_-)} \\ &= \frac{\omega - (\xi_+ + \xi_-)/2 + i\delta[\text{sgn}(\xi_+) + \text{sgn}(\xi_-)]/2 + \hat{d} \cdot \Gamma[(\xi_+ - \xi_-)/2 + i\delta(\text{sgn}(\xi_-) - \text{sgn}(\xi_+))/2]}{(\omega - \xi_+ + i\delta\text{sgn}(\xi_+))(\omega - \xi_- + i\delta\text{sgn}(\xi_-))} \\ &= \frac{\tilde{\omega} + \tilde{d} \cdot \Gamma}{(\omega - \xi_+ + i\delta\text{sgn}(\xi_+))(\omega - \xi_- + i\delta\text{sgn}(\xi_-))}, \end{aligned} \quad (58)$$

where $\tilde{\omega} = \omega - (\xi_+ + \xi_-)/2 + i\delta[\text{sgn}(\xi_+) + \text{sgn}(\xi_-)]/2$ and $\tilde{d} = \hat{d}[(\xi_+ - \xi_-)/2 + i\delta(\text{sgn}(\xi_-) - \text{sgn}(\xi_+))/2]$. Substituting into the formula gives

$$\begin{aligned} f &= -\frac{\pi^2}{3} \epsilon_{ijkl} \int \frac{d^4 k d\omega}{(2\pi)^5} \frac{1}{[(\omega - \xi_+(\mathbf{k}) + i\delta\text{sgn}(\xi_+))(\omega - \xi_-(\mathbf{k}) + i\delta\text{sgn}(\xi_-))]^5} \\ &\quad \times \text{Tr}[(\tilde{\omega} + \tilde{d} \cdot \Gamma)^2 \partial_i(\epsilon(\mathbf{k})\mathbb{I} + d_a\Gamma^a)(\tilde{\omega} + \tilde{d} \cdot \Gamma) \partial_j(\epsilon(\mathbf{k})\mathbb{I} + d_a\Gamma^a)(\tilde{\omega} + \tilde{d} \cdot \Gamma) \partial_k(\epsilon(\mathbf{k})\mathbb{I} + d_a\Gamma^a)(\tilde{\omega} + \tilde{d} \cdot \Gamma) \partial_l(\epsilon(\mathbf{k})\mathbb{I} + d_a\Gamma^a)] \end{aligned} \quad (59)$$

Observe that any term with two or more factors of $\partial\epsilon$ will clearly vanish under the epsilon tensor. The term with one factor of $\partial\epsilon$ can be shown to vanish. The term with no factors of $\partial\epsilon$ gives:

$$\begin{aligned} f &= -\frac{\pi^2}{3} \epsilon_{ijkl} \int \frac{d^4 k d\omega}{(2\pi)^5} \frac{\partial_i d_a \partial_j d_b \partial_k d_c \partial_l d_d}{[(\omega - \xi_+ + i\delta\text{sgn}(\xi_+))(\omega - \xi_- + i\delta\text{sgn}(\xi_-))]^5} \\ &\quad \times \text{Tr}[(\tilde{\omega} + \tilde{d} \cdot \Gamma)^2 \Gamma^a (\tilde{\omega} + \tilde{d} \cdot \Gamma) \Gamma^b (\tilde{\omega} + \tilde{d} \cdot \Gamma) \partial_k \Gamma^c (\tilde{\omega} + \tilde{d} \cdot \Gamma) \Gamma^d] \end{aligned} \quad (60)$$

\mathcal{A}_0 (eV Å)	3.33
\mathcal{B}_0 (eV Å)	2.26
C_0 (eV)	-0.0083
C_1 (eV Å ²)	5.74
C_2 (eV Å ²)	30.4
M_0 (eV)	-0.28
M_1 (eV Å ²)	6.86
M_2 (eV Å ²)	44.5

TABLE I: Parameters of the model Hamiltonian for Bi₂Se₃.

The trace simplifies to $-4\epsilon_{abcd}d^t(\tilde{\omega}^2 - \tilde{d}^2)^2$. Thus:

$$f = 4\frac{\pi^2}{3}\epsilon_{ijkl} \int \frac{d^4k d\omega}{(2\pi)^5} \epsilon_{abcd} d^t \partial_i d_a \partial_j d_b \partial_k d_c \partial_l d_d \frac{1}{[(\omega - \xi_+ + i\delta \text{sgn}(\xi_+))(\omega - \xi_- + i\delta \text{sgn}(\xi_-))]^3} \quad (61)$$

If the chemical potential lies in the conduction band, this is:

$$\begin{aligned} f &= -\frac{\pi^2 i}{4} \epsilon_{ijkl} \int_{BZ \setminus FFS} \frac{d^4k}{(2\pi)^4} \epsilon_{abcd} \frac{d^t \partial_i d_a \partial_j d_b \partial_k d_c \partial_l d_d}{|d|^5} \\ &= -\frac{3}{8\pi^2} \int_{BZ \setminus FFS} d^4k \epsilon_{abcd} \hat{d}^t \partial_x \hat{d}_a \partial_y \hat{d}_b \partial_z \hat{d}_c \partial_\theta \hat{d}_d \end{aligned} \quad (62)$$

If the chemical potential lies in the valence band, we have:

$$f = -\frac{3}{8\pi^2} \int_{FFS} d^4k \epsilon_{abcd} \hat{d}^t \partial_x \hat{d}_a \partial_y \hat{d}_b \partial_z \hat{d}_c \partial_w \hat{d}_d \quad (63)$$

For Bi₂Se₃ with a surface T-breaking field, we have

$$\begin{aligned} \epsilon(\mathbf{k}) &= C_0 + C_1 k_Z^2 + C_2 k_{||}^2, \\ d_1(\mathbf{k}) &= \mathcal{A}_0 k_y \\ d_2(\mathbf{k}) &= -\mathcal{A}_0 k_x \\ d_3(\mathbf{k}) &= m_0 \sin \theta \\ d_4(\mathbf{k}) &= \mathcal{B}_0 k_z \\ d_5(\mathbf{k}) &= -M_0 \cos \theta + M_1 k_z^2 + M_2 k_{||}^2, \end{aligned} \quad (64)$$

where we have only kept terms up to quadratic order in k . The parameters are given in Ref. [2]; we list them in Table I for completeness.

EFFECT OF TOP GATING AT THE SURFACE OF A DOPED TOPOLOGICAL INSULATOR

Here we would like to develop a calculation of the effect of gating at the surface of a doped topological insulator.

We assume that the chemical potential is slightly above the bottom of the conduction band, and that the conduction band bends upward so that at the surface, the chemical potential lies in the bulk band gap. We also assume that a gap m has opened in the Dirac surface states and that the chemical potential is always inside of this gap.

In the simplest depletion length approximation, we assume that within a depletion length z_d from the surface, there are no carriers; if the bulk doping charge density is $-en_b$, where n_b is the bulk carrier density, this means that there is a constant positive charge density en_b in the depletion region. In order to maintain overall charge neutrality, there must be a compensating negative charge near the surface. Let us assume that all of this compensating negative charge comes from the application of a top gate. In practice this is not entirely true, but it may be a good approximation. With such an approximation, we have:

$$V_g C = en_b z_d, \quad (65)$$

where C is the capacitance per unit area of the region between the metallic top gate and the surface of the material.

This negative charge is accumulated in a metal gate a distance d from the surface of the material. Thus, the profile of the charge density is:

$$\rho(z) = -CV_g\delta(z + d) + en_bz, \quad z \leq z_d \quad (66)$$

Note that $z = 0$ is the surface of the material, and $z = -d$ is the position of the top gate. The potential $V(z)$ is therefore given by

$$d^2V/dz^2 = -\rho(z)/(\epsilon(z)\epsilon_0), \quad (67)$$

where $\epsilon(z) = \epsilon_g$ for $-d < z < 0$ is the dielectric constant of the dielectric that is in between the metal gate and the surface of the material, and $\epsilon(z) = \epsilon$ for $z > 0$ is the dielectric constant of the topological insulator.

We are interested in $V(z)$ for $z > 0$. For simplicity, let us assume that $d \approx 0$. The electric field in the region $0 \leq z \leq z_d$ is:

$$E(z) = -\frac{CV_g}{2\epsilon\epsilon_0} + \frac{en_b}{2\epsilon\epsilon_0}z. \quad (68)$$

The potential is then

$$V(z) = -\int_{z_d}^z E(z) dz = -\frac{CV_g}{4\epsilon\epsilon_0}z_d(1 - \frac{z}{z_d})^2 = -\frac{en_g^2}{4\epsilon\epsilon_0 n_b}(1 - \frac{zn_b}{n_g})^2 \quad (69)$$

The potential energy associated with this is $eV(z)$. Note that $z_d = V_gC/en_b = n_g/n_b$, where n_g is the number density of carriers on the top gate.

Thus, we would like to fix the penetration depth of the magnetization, ξ , the gap of the Dirac surface states m (which is induced by the magnetization), and the bulk density n_b , and then study the surface transverse conductance as a function of the gate voltage V_g . For Bi_2Se_3 , we take $\epsilon \approx 100$, so $\epsilon\epsilon_0 \approx 8.8510^{-12} \text{ F/cm}$.

[1] X.-L. Qi, T. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).

[2] C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Phys. Rev. B **82**, 045122 (2010).